TOWARDS OPTIMAL LEARNING OF CHAIN GRAPHS

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ABSTRACT. In this paper, we extend Meek's conjecture (Meek, 1997) from directed and acyclic graphs to chain graphs, and prove that the extended conjecture is true. Specifically, we prove that if a chain graph H is an independence map of the independence model induced by another chain graph G, then (i) G can be transformed into H by a sequence of directed and undirected edge additions and feasible splits and mergings, and (ii) after each operation in the sequence H remains an independence map of the independence model induced by G. Our result has the same important consequence for learning chain graphs from data as the proof of Meek's conjecture in (Chickering, 2002) had for learning Bayesian networks from data: It makes it possible to develop efficient and asymptotically correct learning algorithms under mild assumptions.

1. Preliminaries

In this section, we review some concepts from probabilistic graphical models that are used later in this paper. See, for instance, (Lauritzen, 1996) and (Studený, 2005) for further information. All the graphs and independence models in this paper are defined over a finite set V. All the graphs in this paper are hybrid graphs, i.e. they have (possibly) both directed and undirected edges. We assume throughout the paper that the union and the intersection of sets precede the set difference when evaluating an expression.

If a graph G has a directed (resp. undirected) edge between two nodes X_1 and X_2 , then we write that $X_1 \to X_2$ (resp. $X_1 - X_2$) is in G. When there is a directed or undirected edge between two nodes of G, we say that the two nodes are adjacent in G. The parents of a set of nodes Y of G is the set $Pa_G(Y) = \{X_1 | X_1 \to X_2 \text{ is in } G \text{ and } X_2 \in Y\}$. The neighbors of a set of nodes Y of G is the set $Ne_G(Y) = \{X_1 | X_1 - X_2 \text{ is in } G \text{ and } X_2 \in Y\}$. The boundary of a node X_2 of G is the set $Bd_G(X_2) = Pa_G(X_2) \cup Ne_G(X_2)$. A route between two nodes X_1 and X_n of G is a sequence of nodes X_1, \ldots, X_n st X_i and X_{i+1} are adjacent in G for all $1 \leq i < n$. The length of a route is the number of (not necessarily distinct) edges in the route. We treat all singletons as routes of length zero. A route in G is called undirected if $X_i - X_{i+1}$ is in G for all $1 \leq i < n$. A route in G is called descending from X_1 to X_n if $X_i - X_{i+1}$ or $X_i \to X_{i+1}$ is in G for all $1 \le i < n$. If there is a descending route from X_1 to X_n in G, then X_n is called a descendant of X_1 . Note that X_1 is a descendant of itself, since we allow routes of length zero. The descendants of a set of nodes Y of G is the union of the descendants of each node of Y in G. Given a route ρ between X_1 and X_n in G and a route ρ' between X_n and X_m in G, $\rho \cup \rho'$ denotes the route between X_1 and X_m in G resulting from appending ρ' to ρ .

A chain is a partition of V into ordered subsets, which we call the blocks of the chain. We say that an element $X \in V$ is to the left of another element $Y \in V$ in a chain α if the block of α containing X precedes the block of α containing Y in α . Equivalently, we can say that Y is to the right of X in α . We say that a graph G and a chain α are consistent when (i) for every edge $X \to Y$ in G, X is to the left of Y in α , and (ii) for every edge $X \to Y$ in G, X and Y are in the same block of α . A chain graph (CG) is a graph that is consistent with

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a chain. A set of nodes of a CG is connected if there exists an undirected route in the CG between every pair of nodes of the set. A component of a CG is a maximal (wrt set inclusion) connected set of its nodes. A block of a CG is a set of components of the CG st there is no directed edge between their nodes in the CG. Note that a component of a CG is connected, whereas a block of a CG or a block of a chain that is consistent with a CG is not necessarily connected. Given a set K of components of G, a component $C \in K$ is called maximal in G if none of its nodes is a descendant of $K \setminus \{C\}$ in G. A component C of G is called terminal in G if its descendants in G are exactly C. Let a component C of G be partitioned into two non-empty connected subsets $C \setminus L$ and L. By splitting C into $C \setminus L$ and L in G, we mean replacing every edge X-Y in G st $X\in C\setminus L$ and $Y\in L$ with an edge $X\to Y$. Moreover, we say that the split is feasible if (i) X - Y is in G for all $X, Y \in Ne_G(L) \cap (C \setminus L)$, and (ii) $X \to Y$ is in G for all $X \in Pa_G(L)$ and $Y \in Ne_G(L) \cap (C \setminus L)$. Let L and R denote two components of G st $Pa_G(R) \cap L \neq \emptyset$. By merging L and R in G, we mean replacing every edge $X \to Y$ in G st $X \in L$ and $Y \in R$ with an edge X - Y. Moreover, we say that the merging is feasible if (i) X - Y is in G for all $X, Y \in Pa_G(R) \cap L$, and (ii) $X \to Y$ is in G for all $X \in Pa_G(R) \setminus L$ and $Y \in Pa_G(R) \cap L$.

A section of a route ρ in a CG is a maximal undirected subroute of ρ . A section $X_2 - \ldots - X_{n-1}$ of ρ is a collider section of ρ if $X_1 \to X_2 - \ldots - X_{n-1} \leftarrow X_n$ is a subroute of ρ . Moreover, the edges $X_1 \to X_2$ and $X_{n-1} \leftarrow X_n$ are called collider edges. Let X, Y and Z denote three disjoint subsets of V. A route ρ in a CG is said to be Z-active when (i) every collider section of ρ has a node in Z, and (ii) every non-collider section of ρ has no node in Z. When there is no route in a CG G between a node of X and a node of Y that is Z-active, we say that X is separated from Y given Z in G and denote it as $X \perp_G Y | Z$. We denote by $X \not\perp_G Y | Z$ that $X \perp_G Y | Z$ does not hold.

Let X, Y, Z and W denote four disjoint subsets of V. An independence model M is a set of statements of the form $X \perp_M Y|Z$, meaning that X is independent of Y given Z. Given two independence models M and N, we denote by $M \subseteq N$ that if $X \perp_M Y|Z$ then $X \perp_N Y|Z$. We say that M is a graphoid if it satisfies the following properties: Symmetry $X \perp_M Y|Z \Rightarrow Y \perp_M X|Z$, decomposition $X \perp_M Y \cup W|Z \Rightarrow X \perp_M Y|Z$, weak union $X \perp_M Y \cup W|Z \Rightarrow X \perp_M Y|Z \cup W$, contraction $X \perp_M Y|Z \cup W \wedge X \perp_M W|Z \Rightarrow X \perp_M Y \cup W|Z$, and intersection $X \perp_M Y|Z \cup W \wedge X \perp_M W|Z \cup Y \Rightarrow X \perp_M Y \cup W|Z$. The independence model induced by a CG G, denoted as I(G), is the set of separation statements $X \perp_G Y|Z$. It is known that I(G) is a graphoid (Studený and Bouckaert, 1998, Lemma 3.1). Let H denote the graph resulting from a feasible split or merging in a CG G. Then, H is a CG and I(H) = I(G) (Studený et al., 2009, Lemma 5 and Corollary 9).

A CG G is an independence (I) map of an independence model M if $I(G) \subseteq M$. Moreover, G is a minimal independence (MI) map of M if removing any edge from G makes it cease to be an I map of M. Given any chain C_1, \ldots, C_n that is consistent with G, we say that G satisfies the pairwise block-recursive Markov property wrt M if $X \perp_M Y | \bigcup_{j=1}^{k^*} C_j \setminus \{X, Y\}$ for all non-adjacent nodes X and Y of G and where k^* is the smallest k st $X, Y \in \bigcup_{j=1}^k C_j$. If M is a graphoid and G satisfies the pairwise block-recursive Markov property wrt M, then G is an I map of M (Lauritzen, 1996, Theorem 3.34). We say that a CG G_α is a MI map of an independence model M relative to a chain α if G_α is a MI map of M and G_α is consistent with α .

2. Extension of Meek's Conjecture to Chain Graphs

Given two directed and acyclic graphs G and H st $I(H) \subseteq I(G)$, Meek's conjecture states that we can transform G into H by a sequence of arc additions and covered arc reversals st after each operation in the sequence G is a directed and acyclic graph and $I(H) \subseteq I(G)$ (Meek, 1997). Meek's conjecture was proven to be true in (Chickering, 2002, Theorem 4) by developing an algorithm that constructs a valid sequence of operations. In this section,

Fbsplit(K, L, G)

/* Given a block K of a CG G and a subset L of K, the algorithm repeatedly splits a component of G until L becomes a block of G. Before the splits, the algorithm adds to G the smallest set of edges so that the splits are feasible */

```
1 Let L_1, \ldots, L_n denote the maximal connected subsets of L in G

2 For i=1 to n do

3 Add an edge X-Y to G for all X,Y\in Ne_G(L_i)\cap (K\setminus L)

4 Add an edge X\to Y to G for all X\in Pa_G(L_i) and Y\in Ne_G(L_i)\cap (K\setminus L)

5 For i=1 to n do

6 Let K_j denote the component of G st L_i\subseteq K_j

7 If K_j\setminus L_i\neq\emptyset then

8 Split K_j into K_j\setminus L_i and L_i in G
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Fbmerge(L, R, G)

/* Given two blocks L and R of a CG G, the algorithm repeatedly merges two components of G until $L \cup R$ becomes a block of G. Before the mergings, the algorithm adds to G the smallest set of edges so that the mergings are feasible */

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1 Let R_1, \ldots, R_n denote the components of G that are in R

2 For i=1 to n do

3 Add an edge X-Y to G for all X,Y\in Pa_G(R_i)\cap L

4 Add an edge X\to Y to G for all X\in Pa_G(R_i)\setminus L and Y\in Pa_G(R_i)\cap L

5 For i=1 to n do

6 Let L_j denote the component of G st L_j\subseteq L\cup R and Pa_G(R_i)\cap L_j\neq\emptyset

7 If L_j\neq\emptyset then

8 Merge L_j and R_i in G
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FIGURE 1. Fbsplit and fbmerge.

we extend Meek's conjecture from directed and acyclic graphs to CGs, and prove that the extended conjecture is true. Specifically, given two CGs G and H st $I(H) \subseteq I(G)$, we prove that G can be transformed into H by a sequence of directed and undirected edge additions and feasible splits and mergings st after each operation in the sequence G is a CG and $I(H) \subseteq I(G)$. The proof is constructive in the sense that we give an algorithm that constructs a valid sequence of operations.

We start by introducing two new operations on CGs. It is worth mentioning that all the algorithms in this paper use a "by reference" calling convention, meaning that the algorithms can modify the arguments passed to them. Let K denote a block of a CG G. Let $L \subseteq K$. By feasible block splitting (fbsplitting) K into $K \setminus L$ and L in G, we mean running the algorithm at the top of Figure 1. The algorithm repeatedly splits a component of G until L becomes a block of G. Before the splits, the algorithm adds to G the smallest set of edges so that the splits are feasible. Let L and R denote two blocks of a CG G. By feasible block merging (fbmerging) L and R in G, we mean running the algorithm at the bottom of Figure 1. The algorithm repeatedly merges two components of G until $L \cup R$ becomes a block of G. Before the mergings, the algorithm adds to G the smallest set of edges so that the mergings are feasible. It is worth mentioning that the component L_j in line 6 is guaranteed to be unique by the edges added in lines 3 and 4.

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Go to line 2

Construct $\beta(G, \alpha, \beta)$

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/* Given a CG G and a chain \alpha, the algorithm derives a chain \beta that is consistent with G and as close to \alpha as possible */
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```
1
    Set \beta = \emptyset
 2
    Set H = G
 3 Let C denote any terminal component of H whose leftmost node in \alpha is rightmost in \alpha
    Add C as the leftmost block of \beta
 5
    Let R denote the right neighbor of C in \beta
    If R \neq \emptyset, Pa_G(R) \cap C = \emptyset, and the nodes of C are to the right of the nodes of R in \alpha then
 7
        Replace C, R with R, C in \beta
 8
        Go to line 5
 9
     Remove C and all its incoming edges from H
10
     If H \neq \emptyset then
11
        Go to line 3
     Method B3(G, \alpha)
     /* Given a CG G and a chain \alpha, the algorithm transforms G into G_{\alpha} */
    Construct \beta(G, \alpha, \beta)
 2 Let C denote the rightmost block of \alpha that has not been considered before
 3 Let K denote the leftmost block of \beta st K \cap C \neq \emptyset
    Set L = K \cap C
    If K \setminus L \neq \emptyset then
 5
        Fbsplit(K, L, G)
 7
        Replace K with K \setminus L, L in \beta
 8
     Let R denote the right neighbor of L in \beta
     If R \neq \emptyset and some node of R is not to the right of the nodes of L in \alpha
10
        Fbmerge(L, R, G)
11
        Replace L, R with L \cup R in \beta
12
        Go to line 3
     If \beta \neq \alpha then
13
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FIGURE 2. Method B3.

Our proof of the extension of Meek's conjecture to CGs builds upon an algorithm for efficiently deriving the MI map G_{α} of the independence model induced by a given CG G relative to a given chain α . The pseudocode of the algorithm, called Method B3, can be seen in Figure 2. Method B3 works iteratively by fbsplitting and fbmerging some blocks of G until the resulting CG is consistent with α . It is not difficult to see that such a way of working results in a CG that is an I map of I(G). However, in order to arrive at G_{α} , the blocks of G to modify in each iteration must be carefully chosen. For this purpose, Method B3 starts by calling Construct β to derive a chain β that is consistent with G and as close to α as possible (see lines 5-8). By β being as close to α as possible, we mean that the number of blocks Method B3 will later fbsplit and fbmerge is kept at a minimum, because Method B3 will use β to choose the blocks to modify in each iteration. A line of Construct β that is worth explaining is line 3, because it is crucial for the correctness of Method B3 (see Case 3.2.4 in the proof of Lemma 4). This line determines the order in which the components of

H (initially H = G) are added to β (initially $\beta = \emptyset$). In principle, a component of H may have nodes from several blocks of α . Line 3 labels each terminal component of H with its leftmost node in α and, then, chooses any terminal component whose label node is rightmost in α . This is the next component to add to β .

Once β has been constructed, Method B3 proceeds to transform G into G_{α} . In particular, Method B3 considers the blocks of α one by one in the reverse order in which they appear in α . For each block C of α , Method B3 iterates through the following steps. First, it finds the leftmost block K of β that has some nodes from C. These nodes, denoted as L, are then moved to the right in β by fbsplitting K to create a new block L of G and β . If the nodes of the right neighbor R of L in β are to the right of the nodes of L in α , then Method B3 is done with C. Otherwise, Method B3 moves L further to the right in β by fbmerging L and R in G and β . We prove below that Method B3 is correct. We prove first some auxiliary results.

Lemma 1. Let M denote an independence model, and α a chain C_1, \ldots, C_n . If M is a graphoid, then there exits a unique CG G_{α} that is a MI map of M relative to α . Specifically, for each node X of each block C_k of α , $Bd_{G_{\alpha}}(X)$ is the smallest subset B of $\bigcup_{j=1}^k C_j \setminus \{X\}$ st $X \perp_M \bigcup_{j=1}^k C_j \setminus \{X\} \setminus B|B$.

Proof. Let X and Y denote any two non-adjacent nodes of G_{α} . Let k^* denote the smallest k st $X, Y \in \bigcup_{j=1}^k C_j$. Assume without loss of generality that $X \in C_{k^*}$. Then, $X \perp_M \bigcup_{j=1}^{k^*} C_j \setminus \{X\} \setminus Bd_{G_{\alpha}}(X)|Bd_{G_{\alpha}}(X)$ by construction of G_{α} and, thus, $X \perp_M Y | \bigcup_{j=1}^{k^*} C_j \setminus \{X,Y\}$ by weak union. Then, G_{α} satisfies the pairwise block-recursive Markov property wrt M and, thus, G_{α} is an I map of M. In fact, G_{α} is a MI map of M by construction of $Bd_{G_{\alpha}}(X)$.

Assume to the contrary that there exists another CG H_{α} that is a MI map of M relative to α . Let X denote any node st $Bd_{G_{\alpha}}(X) \neq Bd_{H_{\alpha}}(X)$. Let $X \in C_k$. Then, $X \perp_M \cup_{j=1}^k C_j \setminus \{X\} \setminus Bd_{G_{\alpha}}(X) \mid Bd_{G_{\alpha}}(X)$ and $X \perp_M \cup_{j=1}^k C_j \setminus \{X\} \setminus Bd_{H_{\alpha}}(X) \mid Bd_{H_{\alpha}}(X)$ because G_{α} and H_{α} are MI maps of M. Then, $X \perp_M \cup_{j=1}^k C_j \setminus \{X\} \setminus Bd_{G_{\alpha}}(X) \cap Bd_{H_{\alpha}}(X) \mid Bd_{G_{\alpha}}(X) \cap Bd_{H_{\alpha}}(X)$ by intersection. However, this contradicts the construction of $Bd_{G_{\alpha}}(X)$, because $Bd_{G_{\alpha}}(X) \cap Bd_{H_{\alpha}}(X)$ is smaller than $Bd_{G_{\alpha}}(X)$.

Lemma 2. Let G and H denote two CGs st $I(H) \subseteq I(G)$. For any component C of G, there exists a unique component of H that is maximal in H from the set of components of H that contain a descendant of C in G.

Proof. By definition of CG, there exists at least one such component of H. Assume to the contrary that there exist two such components of H, say K and K'. Note that $Pa_H(K) \cap K' = \emptyset$ and $Pa_H(K') \cap K = \emptyset$ by definition of K and K'. Note also that no node of K or $Pa_H(K)$ is a descendant of K' in H by definition of K. This implies that $K' \perp_H K \cup Pa_H(K) \setminus Pa_H(K')|Pa_H(K')$ and, thus, $K \perp_H K'|Pa_H(K) \cup Pa_H(K')$ by weak union and symmetry.

That K and K' contain some descendants k and k' of C in G implies that there are descending routes from C to k and k' in G st the nodes in the routes are descendant of C in G. Thus, there is a route between k and k' in G st the nodes in the route are descendant of C in G. Note that no node in this route is in $Pa_H(K)$ or $Pa_H(K')$ by definition of K and K'. Then, $K \not\perp_G K' | Pa_H(K) \cup Pa_H(K')$. However, this contradicts the fact that $I(H) \subseteq I(G)$ because, as shown, $K \perp_H K' | Pa_H(K) \cup Pa_H(K')$.

Lemma 3. Let G and H denote two CGs st $I(H) \subseteq I(G)$. Let α denote a chain that is consistent with H. If no descendant of a node X in G is to the left of X in α , then the descendants of X in G are descendant of X in H too.

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¹By convention, $X \perp_M \emptyset | \cup_{j=1}^k C_j \setminus \{X\}$.

Proof. Let D denote the descendants of X in G. Let C denote the component of G that contains X. Note that the descendants of C in G are exactly the set D. Then, there exists a unique component of H that is maximal in H from the set of components of H that contain a node from D, by Lemma 2.

Let K denote the component of H that contains X. Note that K is a component of H that is maximal in H from the set of components of H that contain a node from D, since no node of D is to the left of X in α . It follows from the paragraph above that K is the only such component of H.

We are now ready to prove the correctness of Method B3.

Lemma 4. Let G_{α} denote the MI map of the independence model induced by a CG G relative to a chain α . Then, Method B3(G, α) returns G_{α} .

Proof. We start by proving that Method B3 halts at some point. When Method B3 is done with the rightmost block of α , the rightmost block of β contains all and only the nodes of the rightmost block of α . When Method B3 is done with the second rightmost block of α , the rightmost block of β contains all and only the nodes of the rightmost block of α , whereas the second rightmost block of β contains all and only the nodes of the second rightmost block of α . Continuing with this reasoning, one can see that when Method B3 is done with all the blocks of α , β coincides with α and thus Method B3 halts.

That Method B3 halts at some point implies that it performs a finite sequence of m modifications to G due to the fbsplit and fbmerging in lines 6 and 10. Let G_t denote the CG resulting from the first t modifications to G, and let $G_0 = G$. Specifically, Method B3 constructs G_{t+1} from G_t by either

- adding an edge X Y due to line 3 of Fbsplit or Fbmerge,
- adding an edge $X \to Y$ due to line 4 of Fbsplit or Fbmerge,
- performing all the component splits due to lines 5-8 of Fbsplit, or
- performing all the component mergings due to lines 5-8 of Fbmerge.

Note that none of the modifications above introduces new separation statements. This is trivial to see for the first and second modification. To see it for the third and fourth modification, recall that the splits and the mergings are part of a fbsplit and a fbmerging respectively and, thus, they are feasible. Therefore, $I(G_{t+1}) \subseteq I(G_t)$ for all $0 \le t < m$ and, thus, $I(G_m) \subseteq I(G_0)$.

We continue by proving that G_t is consistent with β for all $0 \le t \le m$. Since this is true for G_0 due to line 1, it suffices to prove that if it is true for G_t then it is true for G_{t+1} for all $0 \le t < m$. We consider the following four cases.

- Case 1: Method B3 constructs G_{t+1} from G_t by adding an edge X Y due to line 3 of Fbsplit or Fbmerge. It suffices to note that X and Y are in the same block of G_t and β .
- Case 2: Method B3 constructs G_{t+1} from G_t by adding an edge $X \to Y$ due to line 4 of Fbsplit. It suffices to note that X is to the left of Y in β , because G_t is consistent with β .
- Case 3: Method B3 constructs G_{t+1} from G_t by adding an edge $X \to Y$ due to line 4 of Fbmerge. Note that X is to the left of R in β , because β is consistent with G_t . Then, X is to the left of L in β , because L is the left neighbor of R in β and $X \notin L$. Then, X is to the left of Y in β , because $Y \in L$.
- Case 4: Method B3 constructs G_{t+1} from G_t by either performing all the component splits due to lines 5-8 of Fbsplit or performing all the component mergings due to lines 5-8 of Fbmerge. Note that the splits and the mergings are feasible, since they are part of a fbsplit and a fbmerging respectively. Therefore, G_{t+1} is a CG. Moreover,

note that β is modified immediately after the fbsplit and the fbmerging so that it is consistent with G_{t+1} .

Note that G_m is not only consistent with β but also with α because, as shown, β coincides with α when Method B3 halts. In order to prove the lemma, i.e. that $G_m = G_\alpha$, all that remains to prove is that $I(G_\alpha) \subseteq I(G_m)$. To see it, note that $G_m = G_\alpha$ follows from $I(G_\alpha) \subseteq I(G_m)$, $I(G_m) \subseteq I(G_0)$, the fact that G_m is consistent with α , and the fact that G_α is the unique MI map of $I(G_0)$ relative to α . Recall that G_α is guaranteed to be unique by Lemma 1, because $I(G_0)$ is a graphoid.

The rest of the proof is devoted to prove that $I(G_{\alpha}) \subseteq I(G_m)$. Specifically, we prove that if $I(G_{\alpha}) \subseteq I(G_t)$ then $I(G_{\alpha}) \subseteq I(G_{t+1})$ for all $0 \le t < m$. Note that this implies that $I(G_{\alpha}) \subseteq I(G_m)$ because $I(G_{\alpha}) \subseteq I(G_0)$ by definition of MI map. First, we prove it when Method B3 constructs G_{t+1} from G_t by either performing all the component splits due to lines 5-8 of Fbsplit or performing all the component mergings due to lines 5-8 of Fbmerge. Note that the splits and the mergings are feasible, since they are part of a fbsplit and a fbmerging respectively. Therefore, $I(G_{t+1}) = I(G_t)$. Thus, $I(G_{\alpha}) \subseteq I(G_{t+1})$ because $I(G_{\alpha}) \subseteq I(G_t)$.

Now, we prove that if $I(G_{\alpha}) \subseteq I(G_t)$ then $I(G_{\alpha}) \subseteq I(G_{t+1})$ when Method B3 constructs G_{t+1} from G_t by adding a directed or undirected edge due to lines 3 and 4 of Fbsplit and Fbmerge. Specifically, we prove that if there is an S-active route ρ_{t+1}^{AB} between two nodes A and B in G_{t+1} , then there is an S-active route between A and B in G_{α} . We prove this result by induction on the number of occurrences of the added edge in ρ_{t+1}^{AB} . We assume without loss of generality that the added edge occurs in ρ_{t+1}^{AB} as few or fewer times than in any other S-active route between A and B in G_{t+1} . We call this the minimality property of ρ_{t+1}^{AB} . If the number of occurrences of the added edge in ρ_{t+1}^{AB} is zero, then ρ_{t+1}^{AB} is an S-active route between A and B in G_t too and, thus, there is an S-active route between A and B in G_t too and, thus, there is an S-active route between A and B in G_t induction hypothesis that the result holds for up to B occurrences of the added edge in B in

Case 1: Method B3 constructs G_{t+1} from G_t by adding an edge X-Y due to line 3 of Fbsplit. Note that X-Y occurs in ρ_{t+1}^{AB} . Assume that X-Y occurs in a collider section of ρ_{t+1}^{AB} . Note that X and Y must be in the same component of G_t for line 3 of Fbsplit to add an edge X-Y. This component also contains a node Z that is in S because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1} . Note that there is a route $X-\ldots-Z-\ldots-Y$ in G_t . Then, we can replace any occurrence of X-Y in a collider section of ρ_{t+1}^{AB} with $X-\ldots-Z-\ldots-Y$, and thus construct an S-active route between A and B in G_{t+1} that violates the minimality property of ρ_{t+1}^{AB} . Since this is a contradiction, X-Y only occurs in non-collider sections of ρ_{t+1}^{AB} . Let $\rho_{t+1}^{AB} = \rho_{t+1}^{AX} \cup X - Y \cup \rho_{t+1}^{YB}$. Note that $X, Y \notin S$ because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1} . For the same reason, ρ_{t+1}^{AX} and ρ_{t+1}^{YB} are S-active in G_{t+1} . Then, there are S-active routes ρ_{α}^{AX} and ρ_{α}^{YB} between A and X and between Y and B in G_{α} by the induction hypothesis.

Let $X - X' - \ldots - Y' - Y$ be a route in G_t st the nodes in $X' - \ldots - Y'$ are in L.⁴ Such a route must exist for line 3 of Fbsplit to add an edge X - Y. Note that X and X' are adjacent in G_{α} since $I(G_{\alpha}) \subseteq I(G_t)$. In fact, $X \to X'$ is in G_{α} . To see it, recall that Method B3 is currently considering the block C of α , and that it has previously considered all the blocks of α to the right of C in α . Then, K only contains nodes from C or from blocks to the left of C in α . However, $X \notin C$ because $X \in K \setminus L$ and $L = K \cap C$. Then, X is to the left of C in α . Thus, $X \to X'$ is in G_{α} because

²Note that maybe A = X and/or Y = B.

³Note that maybe Z = X or Z = Y.

⁴Note that maybe X' = Y'.

 $X' \in L \subseteq C$. Likewise, $Y \to Y'$ is in G_{α} . Note also that $X' - \ldots - Y'$ is in G_{α} . To see it, note that the adjacencies in $X' - \ldots - Y'$ are preserved in G_{α} since $I(G_{\alpha}) \subseteq I(G_t)$. Moreover, these adjacencies correspond to undirected edges in G_{α} , because the nodes in $X' - \ldots - Y'$ are in L and thus in the same block of G_{α} , since $L \subseteq C$. Furthermore, a node in $X' - \ldots - Y'$ is in S because, otherwise, $\rho_{t+1}^{AX} \cup X - X' - \ldots - Y' - Y \cup \rho_{t+1}^{YB}$ would be an S-active route between A and B in G_{t+1} that would violate the minimality property of ρ_{t+1}^{AB} . Then, $\rho_{\alpha}^{AX} \cup X \to X' - \ldots - Y' \leftarrow Y \cup \rho_{\alpha}^{YB}$ is an S-active route between A and B in G_{α} .

Case 2: Method B3 constructs G_{t+1} from G_t by adding an edge $X \to Y$ due to line 4 of Fbsplit. Note that $X \to Y$ occurs in ρ_{t+1}^{AB} . Assume that $X \to Y$ occurs as a collider edge in ρ_{t+1}^{AB} , i.e. $X \to Y$ occurs in a subroute of ρ_{t+1}^{AB} of the form $X \to Y - \ldots - Z \leftarrow W$. Note that a node in $Y - \ldots - Z$ is in S because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1} . Let $X \to X' - \ldots - Y' - Y$ be a route in G_t st the nodes in $X' - \ldots - Y'$ are in L. Such a route must exist for line 4 of Fbsplit to add an edge $X \to Y$. Then, we can replace $X \to Y - \ldots - Z \leftarrow W$ with $X \to X' - \ldots - Y' - Y - \ldots - Z \leftarrow W$ in ρ_{t+1}^{AB} , and thus construct an S-active route between A and B in G_{t+1} that violates the minimality property of ρ_{t+1}^{AB} . Since this is a contradiction, $X \to Y$ never occurs as a collider edge in ρ_{t+1}^{AB} . Let $\rho_{t+1}^{AB} = \rho_{t+1}^{AX} \cup X \to Y \cup \rho_{t+1}^{YB}$. Note that $X, Y \notin S$ because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1} . For the same reason, ρ_{t+1}^{AX} and ρ_{t+1}^{YB} are S-active in G_{t+1} . Then, there are S-active routes ρ_{α}^{AX} and ρ_{α}^{YB} between A and X and between Y and B in G_{α} by the induction hypothesis.

Let $X \to X' - \ldots - Y' - Y$ denote a route in G_t st the nodes in $X' - \ldots - Y'$ are in L.⁸ Such a route must exist for line 4 of Fbsplit to add an edge $X \to Y$. Note that $X' - \ldots - Y'$ is in G_{α} . To see it, note that the adjacencies in $X' - \ldots - Y'$ are preserved in G_{α} since $I(G_{\alpha}) \subseteq I(G_t)$. Moreover, these adjacencies correspond to undirected edges in G_{α} , because the nodes in $X' - \ldots - Y'$ are in L and thus in the same block of G_{α} , since $L \subseteq C$. Furthermore, a node in $X' - \ldots - Y'$ is in S because, otherwise, $\rho_{t+1}^{AX} \cup X \to X' - \ldots - Y' - Y \cup \rho_{t+1}^{YB}$ would be an S-active route between A and B in G_{t+1} that would violate the minimality property of ρ_{t+1}^{AB} . Moreover, note that X and X' are adjacent in G_{α} since $I(G_{\alpha}) \subseteq I(G_t)$. In fact, $X \to X'$ is in G_{α} . To see it, recall that Method B3 is currently considering the block C of α , and that it has previously considered all the blocks of α to the right of C in α . Then, no block to the left of K in β has a node from C or from a block to the right of C in α . Note that X is to the left of K in β , because β is consistent with G_t . Thus, $X \to X'$ is in G_{α} since $X' \in L \subseteq C$. Likewise, note that Y' and Y are adjacent in G_{α} since $I(G_{\alpha}) \subseteq I(G_t)$. In fact, $Y' \leftarrow Y$ is in G_{α} . To see it, note that K only contains nodes from C or from blocks to the left of C in α . However, $Y \notin C$ because $Y \in K \setminus L$ and $L = K \cap C$. Then, Y is to the left of C in α . Thus, $Y' \leftarrow Y$ is in G_{α} because $Y' \in L \subseteq C$. Then, $\rho_{\alpha}^{AX} \cup X \to X' - \ldots - Y' \leftarrow Y \cup \rho_{\alpha}^{YB}$ is an S-active route between A and B in G_{α} .

Case 3: Method B3 constructs G_{t+1} from G_t by adding an edge X-Y due to line 3 of Fbmerge. Note that X-Y occurs in ρ_{t+1}^{AB} . We consider two cases.

Case 3.1: Assume that X-Y occurs in a collider section of ρ_{t+1}^{AB} . Let $\rho_{t+1}^{AB} = \rho_{t+1}^{AZ} \cup Z \to X' - \ldots - X - Y - \ldots - Y' \leftarrow W \cup \rho_{t+1}^{WB,9}$ Note that $Z,W \notin S$ because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1} . For the same reason,

⁵Note that maybe A = X and/or Y = B.

⁶Note that maybe Y = Z and/or W = X.

⁷Note that maybe X' = Y'.

⁸Note that maybe X' = Y'.

⁹Note that maybe A = Z, X' = X, Y' = Y, W = Z and/or W = B.

 ρ_{t+1}^{AZ} and ρ_{t+1}^{WB} are S-active in G_{t+1} . Then, there are S-active routes ρ_{α}^{AZ} and ρ_{α}^{WB} between A and Z and between W and B in G_{α} by the induction hypothesis. Let R_i denote the component of G_t in R that Fbmerge is processing when the edge X-Y gets added. Recall that Method B3 is currently considering the block C of α , and that it has previously considered all the blocks of α to the right of C in α . Then, R_i only contains nodes from C or from blocks to the left of C in α . In other words, $R_i \subseteq \bigcup_{j=1}^{k^*} C_j \setminus \{X,Y\}$ where $C_{k^*} = C$ (recall that $X,Y \in L \subseteq C$). Therefore, $X \not\perp_{G_t} Y | \bigcup_{j=1}^{k^*} C_j \setminus \{X,Y\}$ because X and Y must be in $Pa_{G_t}(R_i)$ for line 3 of Fbmerge to add an edge X-Y. Then, X and Y are adjacent in G_{α} because, otherwise, $X \perp_{G_{\alpha}} Y | \bigcup_{j=1}^{k^*} C_j \setminus \{X,Y\}$ which would contradict that $I(G_{\alpha}) \subseteq I(G_t)$. In fact, X-Y is in G_{α} because X and Y are in the same block of α , since $X,Y \in L \subseteq C$.

Note that $X'-\ldots-X$ and $Y-\ldots-Y'$ are in G_{α} . To see it, note that the adjacencies in $X'-\ldots-X$ and $Y-\ldots-Y'$ are preserved in G_{α} since $I(G_{\alpha})\subseteq I(G_t)$. Moreover, these adjacencies correspond to undirected edges in G_{α} , because the nodes in $X'-\ldots-X$ and $Y-\ldots-Y'$ are in L since $X,Y\in L$ and, thus, they are in the same block of G_{α} since $L\subseteq C$. Then, $X'-\ldots-X-Y-\ldots-Y'$ is in G_{α} . Furthermore, a node in $X'-\ldots-X-Y-\ldots-Y'$ is in S because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1} . Note also that Z and X' are adjacent in G_{α} since $I(G_{\alpha})\subseteq I(G_t)$. In fact, $Z\to X'$ is in G_{α} . To see it, recall that Method B3 is currently considering the block C of C on C and that it has previously considered all the blocks of C to the right of C in C. Then, no block to the left of C in C

Case 3.2: Assume that X - Y occurs in a non-collider section of ρ_{t+1}^{AB} . Note that this implies that G_t has a descending route from X to A or to a node in S, or from Y to B or to a node in S. Assume without loss of generality that G_t has a descending route from Y to B or to a node in S.

Let R_i denote the component of G_t in R that Fbmerge is processing when the edge X-Y gets added. Let L_Y denote the component of G_t that contains the node Y. Let D denote the component of G_{α} that is maximal in G_{α} from the set of components of G_{α} that contain a descendant of L_Y in G_t . Recall that D is guaranteed to be unique by Lemma 2, because $I(G_{\alpha}) \subseteq I(G_t)$. We now show that some $d \in D$ is a descendant of R_i in G_t . We consider four cases.

- Case 3.2.1: Assume that $D \cap L_Y \neq \emptyset$. It suffices to consider any $d \in R_i$. To see it, recall that Method B3 is currently considering the block C of α , and that it has previously considered all the blocks of α to the right of C in α . Then, R_i only contains nodes from C or from blocks to the left of C in α . Thus, d is not to the right of the nodes of $D \cap L_Y$ in α , since $L_Y \subseteq L \subseteq C$. Moreover, d is not to the left of the nodes of $D \cap L_Y$ in α because, otherwise, there would be a contradiction with the definition of D. Then, $d \in D$.
- Case 3.2.2: Assume that $D \cap L_Y = \emptyset$ and $D \cap R_i \neq \emptyset$. It suffices to consider any $d \in D \cap R_i$.
- Case 3.2.3: Assume that $D \cap L_Y = \emptyset$, $D \cap R_i = \emptyset$, and some $d \in D$ was a descendant of some $r \in R_i$ in G_0 . Recall that Method B3 is currently considering the block C of α , and that it has previously considered all the blocks of α to the right of C in α . Then, R_i only contains nodes from

C or from blocks to the left of C in α . Then, r was not in the blocks of α previously considered, since $r \in R_i$. Therefore, no descendant of r in G_0 is currently to the left of r in β and, thus, the descendants of r in G_0 are descendant of r in G_t by Lemma 3, because $I(G_t) \subseteq I(G_0)$ and β is consistent with G_t . Then, d is a descendant of r and thus of R_i in G_t .

Case 3.2.4: Assume that $D \cap L_Y = \emptyset$, $D \cap R_i = \emptyset$, and no node of D was a descendant of a node of R_i in G_0 . As shown in Case 3.2.3, the descendants of any node $r \in R_i$ in G_0 are descendant of r in G_t too. Therefore, no descendant of r in G_0 was to the left of the nodes of D in α because, otherwise, a descendant of r and thus of L_Y in G_t would be to the left of the nodes of D in α , which would contradict the definition of D. Recall that no descendant of r in G_0 was in D either. Note also that the nodes of D are to the left of the nodes of R_i in α , by definition of D and the fact that $D \cap R_i =$ Ø. These observations have two consequences. First, the components of G containing a node from D were still in H when any component of Gcontaining a node from R_i became a terminal component of H in Construct β . Thus, Construct β added the components of G containing a node from D to β after having added the components of G containing a node from R_i . Second, Construct β did not interchange in β any component of G containing a node from D with any component of G containing a node from R_i .

Recall that Method B3 is currently considering the block C of α , and that it has previously considered all the blocks of α to the right of C in α . Note that the nodes of D were not in the blocks of α previously considered because, otherwise, C and thus the nodes of L_Y (recall that $L_Y \subseteq L \subseteq C$) would be to the left of D in α , which would contradict the definition of D. Therefore, the nodes of D are currently still to the left of R_i in β . Note that the only component to the left of R_i in β that contains a descendant of L_Y in G_t is precisely L_Y , because L is the left neighbor of R in β , $L_Y \subseteq L$, and β is consistent with G_t . However, $D \cap L_Y = \emptyset$. Thus, D contains no descendant of L_Y in G_t , which contradicts the definition of D. Thus, this case never occurs.

We continue with the proof of Case 3.2. Let $\rho_{t+1}^{AB} = \rho_{t+1}^{AX} \cup X - Y \cup \rho_{t+1}^{YB}$. Note that $X,Y \notin S$ because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1} . For the same reason, ρ_{t+1}^{AX} and ρ_{t+1}^{YB} are S-active in G_{t+1} . Note that X and Y must be in $Pa_{G_t}(R_i)$ for line 3 of Fbmerge to add an edge X-Y. Then, no descendant of R_i in G_t is in S because, otherwise, there would be an S-active route ρ_t^{XY} between X and Y in G_t and, thus, $\rho_{t+1}^{AX} \cup \rho_t^{XY} \cup \rho_{t+1}^{YB}$ would be an S-active route between A and B in G_{t+1} that would violate the minimality property of ρ_{t+1}^{AB} . Then, there is an S-active descending route ρ_t^{rd} from some $r \in R_i$ to some $d \in D$ in G_t because, as shown, D contains a descendant of R_i in G_t . Then, $\rho_{t+1}^{AX} \cup X \to X' - \ldots - r \cup \rho_t^{rd}$ is an S-active route between A and A in A-active route between A-and A-active route between A-and A-active route between A-and A-active route between A-active route A-active route between A-active route A-active route A-active route A-a

Recall that we assumed without loss of generality that G_t has a descending route from Y to a node E st E = B or $E \in S$. Note that E is a descendant of L_Y in

¹⁰Note that maybe A = X and/or Y = B.

¹¹Note that maybe X' = r.

¹²Note that maybe Y' = r.

 G_t and, thus, E is a descendant of d in G_{α} by definition of D and the fact that $d \in D$. Let ρ_{α}^{dE} denote the descending route from d to E in G_{α} . Assume without loss of generality that G_{α} has no descending route from d to B or to a node of S that is shorter than ρ_{α}^{dE} . We now consider two cases.

- Case 3.2.5: Assume that E = B. Note that ρ_{α}^{dE} is S-active in G_{α} by definition and the fact that $d \notin S$. To see the latter, recall that no descendant of R_i in G_t (among which is d) is in S. Thus, $\rho_{\alpha}^{Ad} \cup \rho_{\alpha}^{dE}$ is an S-active route between A and B in G_{α} .
- Case 3.2.6: Assume that $E \in S$. Let ρ_{α}^{dB} and ρ_{α}^{Ed} denote the routes resulting from reversing ρ_{α}^{Bd} and ρ_{α}^{dE} . Consider the route $\rho_{\alpha}^{Ad} \cup \rho_{\alpha}^{dB}$ between A and B in G_{α} . If this route is S-active, then we are done. If it is not S-active in G_{α} , then d occurs in a collider section of $\rho_{\alpha}^{Ad} \cup \rho_{\alpha}^{dB}$ that has no node in S. Then, we can replace each such occurrence of d with $\rho_{\alpha}^{dE} \cup \rho_{\alpha}^{Ed}$ and, thus construct an S-active route between A and B in G_{α} .
- Case 4: Method B3 constructs G_{t+1} from G_t by adding an edge $X \to Y$ due to line 4 of Fbmerge. Note that $X \to Y$ occurs in ρ_{t+1}^{AB} . We consider two cases.
 - Case 4.1: Assume that $X \to Y$ occurs as a collider edge in ρ_{t+1}^{AB} . Let $\rho_{t+1}^{AB} = \rho_{t+1}^{AX} \cup X \to Y \cup \rho_{t+1}^{YB}$. Note that $X \notin S$ because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1} . For the same reason, ρ_{t+1}^{AX} is S-active in G_{t+1} . Then, there is an S-active route ρ_{α}^{AX} between A and X in G_{α} by the induction hypothesis. Let R_i denote the component of G_t in R that Fbmerge is processing when the edge $X \to Y$ gets added. Recall that Method B3 is currently considering the block C of α , and that it has previously considered all the blocks of α to the right of C in α . Then, R_i only contains nodes from C or from blocks to the left of C in α . In other words, $R_i \subseteq \bigcup_{j=1}^{k^*} C_j \setminus \{X,Y\}$ where k^* is the smallest k st $X,Y \in \bigcup_{j=1}^k C_j$ (recall that $Y \in L \subseteq C$). Therefore, $X \not\perp_{G_t} Y | \bigcup_{j=1}^{k^*} C_j \setminus \{X,Y\}$ because X and Y must be in $Pa_{G_t}(R_i)$ for line 4 of Fbmerge to add an edge $X \to Y$. Then, X and Y are adjacent in G_{α} because, otherwise, $X \perp_{G_{\alpha}} Y | \bigcup_{j=1}^{k^*} C_j \setminus \{X,Y\}$ which would contradict that $I(G_{\alpha}) \subseteq I(G_t)$. In fact, $X \to Y$ is in G_{α} . To see it, recall that Method B3 is currently considering the block C of α , and that it has previously considered all the blocks of α to the right of C in α . Then, no block to the left of L in β has a node from C or from a block to the right of C in α . Note that X is to the left of R in β , because β is consistent with G_t . Then, X is to the left of L in β , because L is the left neighbor of R in β and $X \notin L$. Thus, $X \to Y$ is in G_{α} because $Y \in L \subseteq C$. We now consider two cases.
 - Case 4.1.1: Assume that $\rho_{t+1}^{YB} = Y \ldots Y \leftarrow X \cup \rho_{t+1}^{XB}$. Note that a node in $Y \ldots Y$ is in S because, otherwise, ρ_{t+1}^{AB} would not be S-active in G_{t+1} . For the same reason, ρ_{t+1}^{XB} is S-active in G_{t+1} . Then, there is an S-active route ρ_{α}^{XB} between X and B in G_{α} by the induction hypothesis. Note that $Y \ldots Y$ is in G_{α} . To see it, note that the adjacencies in $Y \ldots Y$ are preserved in G_{α} since $I(G_{\alpha}) \subseteq I(G_t)$. Moreover, these adjacencies correspond to undirected edges in G_{α} , because the nodes in $Y \ldots Y$ are in L since $Y \in L$ and, thus, they are in the same block of G_{α} since $L \subseteq C$. Then, $\rho_{\alpha}^{AX} \cup X \to Y \ldots Y \leftarrow X \cup \rho_{\alpha}^{XB}$ is an S-active route between A and B in G_{α} .
 - Case 4.1.2: Assume that $\rho_{t+1}^{YB} = Y \ldots Z \leftarrow W \cup \rho_{t+1}^{WB}$. Note that $W \notin S$ and a node in $Y \ldots Z$ is in S because, otherwise, ρ_{t+1}^{AB} would

¹³Note that maybe A = X and/or Y = B.

¹⁴Note that maybe Y = Z, W = X and/or W = B. Note that $Y \neq Z$ or $W \neq X$, because the case where Y = Z and W = X is covered by Case 4.1.1.

Method G2H(G, H)

/* Given two CGs G and H st $I(H) \subseteq I(G)$, the algorithm transforms G into H by a sequence of directed and undirected edge additions and feasible splits and mergings st after each operation in the sequence G is a CG and $I(H) \subseteq I(G)$ */

- 1 Let α denote a chain that is consistent with H
- 2 Method B3(G, α)
- 3 Add to G the edges that are in H but not in G

FIGURE 3. Method G2H.

not be S-active in G_{t+1} . For the same reason, ρ_{t+1}^{WB} is S-active in G_{t+1} . Then, there is an S-active route ρ_{α}^{WB} between W and B in G_{α} by the induction hypothesis. Note that $Y - \ldots - Z$ is in G_{α} . To see it, note that the adjacencies in $Y - \ldots - Z$ are preserved in G_{α} since $I(G_{\alpha}) \subseteq I(G_t)$. Moreover, these adjacencies correspond to undirected edges in G_{α} , because the nodes in $Y - \ldots - Z$ are in L since $Y \in L$ and, thus, they are in the same block of G_{α} since $L \subseteq C$. Moreover, note that Z and W are adjacent in G_{α} since $I(G_{\alpha}) \subseteq I(G_t)$. In fact, $Z \leftarrow W$ is in G_{α} . To see it, recall that no block to the left of L in β has a node from C or from a block to the right of C in α . Note that W is to the left of L in β , because β is consistent with G_t . Thus, $Z \leftarrow W$ is in G_{α} since $Z \in L \subseteq C$. Then, $\rho_{\alpha}^{AX} \cup X \rightarrow Y - \ldots - Z \leftarrow W \cup \rho_{\alpha}^{WB}$ is an S-active route between A and B in G_{α} .

Case 4.2: Assume that $X \to Y$ occurs as a non-collider edge in ρ_{t+1}^{AB} . The proof of this case is the same as that of Case 3.2, with the only exception that X - Y should be replaced by $X \to Y$.

We are now ready to prove the main result of this paper, namely that the extension of Meek's conjecture to CGs is true. The proof is constructive in the sense that we give an algorithm that constructs a valid sequence of operations. The pseudocode of our algorithm, called Method G2H, can be seen in Figure 3. The following theorem proves that Method G2H is correct.

Theorem 1. Given two CGs G and H st $I(H) \subseteq I(G)$, Method G2H(G, H) transforms G into H by a sequence of directed and undirected edge additions and feasible splits and mergings st after each operation in the sequence G is a CG and $I(H) \subseteq I(G)$.

Proof. Note from line 1 that α denotes a chain that is consistent with H. Let G_{α} denote the MI map of I(G) relative to α . Recall that G_{α} is guaranteed to be unique by Lemma 1, because I(G) is a graphoid. Note that $I(H) \subseteq I(G)$ implies that G_{α} is a subgraph of H. To see it, note that $I(H) \subseteq I(G)$ implies that we can obtain a MI map of I(G) relative to α by just removing edges from H. However, G_{α} is the only MI map of I(G) relative to α .

Then, it follows from the proof of Lemma 4 that line 2 transforms G into G_{α} by a sequence of directed and undirected edge additions and feasible splits and mergings, and that after each operation in the sequence G is a CG and $I(G_{\alpha}) \subseteq I(G)$. Thus, after each operation in the sequence $I(H) \subseteq I(G)$ because $I(H) \subseteq I(G_{\alpha})$ since, as shown, G_{α} is a subgraph of H. Finally, line 3 transforms G from G_{α} to H by a sequence of edge additions. Of course, after each edge addition G is a CG and $I(H) \subseteq I(G)$ because G_{α} is a subgraph of H.

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